Acta Physicae Superficierum · Vol II · 1990

SPIN POLARIZATION OF LOW ENERGY ELECTRONS SCATTERED FROM MAGNETIC Ni(110) SURFACES*

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ABSTRACT. The continuation of an analytical approach to elastic spin polarized low energy electron diffraction (SPLEED) [1] from magnetic surfaces is presented and searched numerically using three different layer dependent surface magnetization models of the Ni(110) surfaces case. In the approach, the dynamical surface scattering LEED and exchange potentials are expressed in terms of the effective scattering potentials of a free atom. The SPLEED exchange scattering asymmetry during the reversal of the polarization direction of the incident electron beam are given in analytical form and the asymmetry effects are computed numerically. The temperature dependence of the surface polarization effect for nickel surfaces is presented graphically. The obtained results correspond to those of experiments and literature.

I. INTRODUCTION

The understanding of the physics of ferromagnetism continues to challenge theoretists as well as experimentalists. In particular, surface ferromagnetism has been the subject of increasing interest in recent years because it allows to study the influence of reduced dimensionality on structural and magnetic phase transitions and critical phenomena [2]. The recent increase in activity in the area of surface magnetism is a consequence of new spin-sensitive surface spectroscopies and the implementation of powerful new techniques for calculating spin dependent surface band structure. The study of surface magnetism requires a spectroscopy with extreme surface specificity in order to isolate effects associated with the properties of the surface layer from those associated with subsurface layers. This is especially true in the case of thin films, which provide the opportunity to study the magnetic properties of quasi-two-dimensional systems [3].

In the literature, several spin-sensitive surface spectroscopies have been described. They have been developed on the basis of field emission [4] and photoemission [5]. In photoemission, however, the photoelectrons ejected from

* This work was carried out within the problem CPBP 01.08.

the surface layer are often difficult to distinguish from those that originate in subsurface layers. Frequently the ejected electrons will originate in up to ten or more layers beneath the surface.

Other spectroscopies which have been developed make use of incident beams of polarized electrons; here belong spin polarized low energy diffraction (SPLEED), spin polarized inverse photoelectron spectroscopy and spin polarized low energy electron loss spectroscopy [6]. These spectroscopies are more surface specific because incident low energy electrons do not penetrate far into the surface and thus give us an information about the local properties of the surface. Particularly interesting and useful phenomena occur when the incident electron beam is polarized, i.e., when the number of electrons with spin parallel to a preferential direction differs from the number with spin antiparallel. The polarized low energy electron beam interacting with the surface system *via* exchange or spin-orbit coupling produces diffracted polarized beams, the polarization of which is a unique quantity for studing magnetic, electronic and even geometrical surface properties.

The question how the scattering of an electron from magnetic surfaces depends on the orientation of its spin with respect to the surface magnetization has first been raised by Davisson and Germer [7], who attempted to observe spin polarized electron scattering in a double scattering experiment using Ni(111)-surfaces. According to their analysis, they could not detect the effect. A reinterpretation by Kuyat [8] implied that Davisson and Germer's data contained exchange-induced magnetic scattering asymmetries of up 27%. However, Feder [9], on the basis of theoretical calculations, suggested that the data could also be explained by small misalignment of the crystal

In the light of recent experimental results on Ni(001) surfaces [2], where the exchange-induced scattering asymmetry amounted to several percent, it was clear that Davisson and Germer did not detect a magnetic effect in electron scattering.

Today, more than half a century after Davisson and Germer, it still remains a challenging task to use spin-polarized low energy electron diffraction for the magnetic analysis of surfaces, just like conventional LEED for their structural analysis. The final aim is the quantitative analysis of space dependent spin densities from quantitative comparison of relativistic dynamical scattering calculations with SPLEED experiments. The first steps in this direction were done by theory, starting with a kinematical approach [10] and a first dynamical study [11]. Experiments in the field became possible only after the introduction of the GaAs-source for the spin polarized electrons [12], starting with the pioneering SPLEED experiment of Celotta *et al.* [13].

The merit of SPLEED, by comparison with other probes of surface magnetism, is due to its general applicability to any ferromagnetic surface and its ability to give information on just the few topmost atomic layers, for which

deviation from the bulk magnetization must be considered in the ground state. Furthermore, the use of low energy electrons allow to obtain by the direct measurement the magnetic moments in ferromagnetic films [14].

For comparison with extended modern theoretical work on the ground state, we need low temperature experiments. For 3*d*-ferromagnets, however, because of their high Curie temperatures, room temperature experiments can be considered to be a reasonable approximation of low temperature ones.

When low energy primary electrons strike a metal surface, several processes take place, such as elastic scattering and inelastic scattering due to excitation of single electrons and of collective modes. The inelastic scattering gives rise to the characteristic energy loss spectrum, whose peaks correspond to the characteristic electronic excitation energies of the metal. If the surface exhibits ferromagnetic order, the exchange interaction as well as the magnetic dipole-dipole interaction between the incident electron and the magnetic ground state electrons depend on the spin orientation of the incident electron relative to the magnetization axis. Since the dipole-dipole term is negligible for low energy electron diffraction, one is left with two spin dependent parts in the effective scattering potential: the spin-orbit term and the exchange term. In the case of a material like nickel, where both terms are comparable, the neglect of spin-orbit coupling might still be acceptable provided that the magnetization axis is placed in the scattering plane chosen so as to coincide with a mirror plane. This is the case of electron diffraction from the (110) surfaces of the nickel crystal structure. In this case the scattering asymmetry in the direction normal to the plane is determined by spin-orbit coupling, while the in-plane asymmetry is caused by magnetic exchange scattering.

Both spin-orbit interaction and, in the case of magnetically ordered surfaces exchange interaction, can give rise to spin dependent effects in SPLEED experiments. The physical basis of the spin dependence in elastic scattering can easily be visualised for the case of electron scattering from free atoms. For motion in a central potential $V(\vec{r})$, the spin-orbit term in the interaction Hamiltonian can be written as

$$V_{so}(\vec{r}) = \frac{1}{2mc^2} \frac{1}{r} \frac{dV}{dr} \vec{S} \cdot \vec{L} \tag{1.1}$$

where $\vec{S}$ is the spin vector of the incident electron and $\vec{L}$ is its orbital angular momentum with respect to the scattering centre. If we regard an unpolarized incident beam of energy E as consisting of equal numbers of electrons with spin up ($\uparrow$) and spin down ($\downarrow$) relative to the scattering plane, these electrons experience different scattering potentials as a consequence of $V_{so}(\vec{r})$. Thus, the numbers of spin up and spin down electrons scattered in a particular direction θ relative to the incident beam, $N^{\uparrow}(E, \theta)$ and $N^{\downarrow}(E, \theta)$, will not in general be the same, i.e., the corresponding differential scattering cross-section $\sigma^{\uparrow}(E, \theta)$ and $\sigma^{\downarrow}(E, \theta)$ are different. Since $N^{\uparrow}(E, \theta)$ and $N^{\downarrow}(E, \theta)$ are proportional to the corresponding

cross-sections, unpolarized electrons elastically scattered through θ are polarized to a degree amounting to

$$P(E,\theta)=\frac{\sigma^{\uparrow}(E,\theta)-\sigma^{\downarrow}(E,\theta)}{\sigma^{\uparrow}(E,\theta)+\sigma^{\downarrow}(E,\theta)}. \tag{1.2}$$

The differences on $\sigma^{\uparrow}(E,\theta)$ and $\sigma^{\downarrow}(E,\theta)$ also lead to spin dependences in the scattering of a polarized incident beam (see next sections). Thus spin dependence is characterized by an asymmetry parameter

$$A(E,\theta)=\frac{1}{P_0}\frac{I^{\uparrow}(E,\theta)-I^{\downarrow}(E,\theta)}{I^{\uparrow}(E,\theta)+I^{\downarrow}(E,\theta)}, \tag{1.3}$$

where $I^{\uparrow}(E,\theta)$ and $I^{\downarrow}(E,\theta)$ are the scattered electron currents at angle θ for incident electrons with spin-up and spin-down, respectively. $1/P_0$ is a normalization factor accounting for the fact that the magnitude of the incident beam polarization P_0 is in general less than unity.

It is important to note that, to a good approximation, the measured values of A and P will be independent of the instrument response function. This is due to the fact that they are absolute ratios. The instrument response function, which appears in both the numerator and denominator, cancels out point by point. This is in marked contrast to LEED intensity measurements where the data have to be corrected for a response function that is generally very difficult to determine.

Early SPLEED measurements focussed on materials of relatively high Z, for which spin-orbit coupling is strong. However, lower-Z surfaces have also been shown to be accessible to SPLEED investigation, despite the fact that the magnitudes of the features observed in $P(E)$ and $A(E)$ dependences are generally rather small.

Our present paper is a continuation of the analytical approach to the problem to which we have devoted Refs. [1]. In those papers we have derived a temperature and spin dependent interaction potential for electrons scattered from magnetic surfaces. Here we describe shortly the surface many-body systems of the bound polarized electrons (Sec. II) as well as the principles of elastic spin polarized low energy electron diffraction (Sec. III). Next, in Section IV we write the spin dependent scattering potentials discussed in Refs. [1] in a more elaborate form obtained recently, and we use them for the numerical computation of the temperature dependences of the spin polarization of the electrons scattered from magnetic surfaces (Sec. V).

II. MAGNETIC SURFACE MANY-ELECTRON SYSTEMS

In this section we describe the bound polarized electrons, which are part of the surface system and determine its magnetic structure both in the zero temperature ground state and at higher temperatures.

We recall that one of the most important advances in the determination of the electronic and magnetic structure of materials, was the development of density functional theory by Hohenberg and Kohn [12] and its spin-polarized extentions [15]. The basic result is the proof by Hohenberg and Kohn that the ground state energy of a many-body system is a unique functional of the density, $n(\vec{r})$, and is minimal when calculated for the true ground state density.

To describe a ferromagnetically ordered system relativistically let us define the interaction of a Dirac particle of mass m and charge e with the electromagnetic field H_{int} [15, 16]

$$H_{\text{int}} = (1/c) \int d^3 r J_\mu A^\mu , \tag{2.1}$$

where the four-current operator J^μ and four-potential A^μ are given by

$$\underline{\hat{J}} = (c\hat{\rho}, \underline{J}_0) = ec \hat{\bar{\Psi}}(\vec{r}) \gamma^\mu \hat{\Psi}(\vec{r}) , \tag{2.2}$$

$$\underline{A} = (\varphi, \vec{A}_{\text{ext}}) , \tag{2.3}$$

and c denotes the light velocity, whereas γ^μ are Dirac matrices and stands for the Dirac four-spinors. It has been shown [15] that the Hohenberg-Kohn theorems can be generalized to include relativistic effects and that in such a case one can obtain the one-particle Dirac equation [17]

$$\{c\vec{\alpha} \cdot [\vec{p} - (e/c) \vec{A}_{\text{eff}}(\vec{r})] + eV_{\text{eff}}(\vec{r})\} \Phi_i(\vec{r}) = E_i \Phi_i(\vec{r}) , \tag{2.4}$$

where the effective potentials are given by

$$V_{\text{eff}}(\vec{r}) = \varphi(\vec{r}) + e \int \frac{n(\vec{r}) d^3 r'}{|\vec{r} - \vec{r}'|} + \frac{\delta E_{\text{xc}}[\underline{J}_\mu]}{\delta \underline{J}_0(\vec{r})} , \tag{2.5}$$

$$\vec{A}_{\text{eff}}(\vec{r}) = \vec{A}_{\text{ext}} \frac{\delta E_{\text{xc}}[\underline{J}_\mu]}{\cdot \underline{J}_0(\vec{r})} , \tag{2.6}$$

and $[n(\vec{r}) V]$ is the number density. The exchange and correlation energy functional $E_{\text{xc}}[\underline{J}_\mu]$ contains magnetic effects through its dependence on the spatial components of the current.

If we are interested in spin effects this approach has to be generalized. Following McDonald and Vosko [18] we take the non-relativistic viewpoint that the external fields couple to the particle and spin densities. Defining the magnetization density by

$$\vec{m}(\vec{r}) = \mu_B \hat{\bar{\Psi}} \vec{\sigma} \hat{\Psi} , \tag{2.7}$$

where $\vec{\sigma}$ stands for the vector of the spin operator, and the external Hamiltonian can be written as

$$H_{\text{ext}} = \int d^3 r [\hat{\rho}(\vec{r}) \Phi(\vec{r}) - \vec{m}(\vec{r}) \cdot \vec{B}] . \tag{2.8}$$

The first term contains the usual minimal electromagnetic coupling while the second term represents coupling to the magnetic dipole moment.

This external Hamiltonian leads to single-particle Dirac equations of the form

$$\{c\vec{\alpha}\cdot\vec{p}+eV_{\text{eff}}(\vec{r})-\mu_B\vec{\Sigma}\cdot U_{\text{eff}}(\vec{r})\}\,\Phi_i(\vec{r})=E_i\,\Phi_i(\vec{r})\,, \tag{2.9}$$

where $U_{\text{eff}}(\vec{r})$ and the spin density operator $\vec{\Sigma}$ are given by

$$U_{\text{eff}}(\vec{r})=\vec{B}+\frac{\delta E[J_\mu]}{\delta\vec{m}(\vec{r})}\,, \tag{2.10}$$

$$\vec{\Sigma}=\begin{pmatrix}\vec{\sigma} & 0\\ 0 & -\vec{\sigma}\end{pmatrix}, \tag{2.11}$$

and $\vec{\sigma}$ denotes the usual 2×2 Pauli spinors, and the number density $n(\vec{r})$ and magnetization density are given by

$$n(\vec{r})=\sum_i \Phi_i^+(\vec{r})\,\Phi_i(\vec{r})\,, \tag{2.12}$$

$$\vec{m}(\vec{r})=\mu_B\sum_i \Phi_i^+(\vec{r})\,\vec{\Sigma}\Phi_i(\vec{r})\,. \tag{2.13}$$

The sums run over all occupied states.

Taking the relativistic limit of the Dirac equation and retaining the first relativistic correction, we obtain a Pauli-like equation for magnetic field coupling to the spin only

$$\{[p^2/2m-p^4/8m^3c^2]-\mu_B\vec{\sigma}\cdot[\vec{B}-\vec{\nabla}(\vec{\nabla}\times\vec{p})/2mc]+[eV+e\hbar^2\nabla^3/8m^2c^2]\}\,\Psi$$
$$=(E-mc^2)\,\Psi\,. \tag{2.14}$$

In this equation, $\vec{B}$ and V are the effective magnetic fields and potentials, respectively, which include the effects of exchange and correlation.

The set of self-consistent equations (2.5) and (2.9–2.13) fully determines the correct charge and magnetization of a many-body problem of the system reduced to the effective one-particle problem. If one knew the exact E_{xc}, one would have a solution of the many-electron problem. However, these functionals are not known and some approximations are used.

A great advantage of the spin-density functional method is that it gives us an approximate form of the exchange and correlation functional, reducing the many-body electrons problem to a single-particle problem.

Since our treatment is devoted to surface systems as they stand in any spin polarized low energy electron spectroscopy we now describe, as a next problem, the most successful structural models currently used for *ab initio* surface calculations.

One of the most successful structural models for surface calculations is the thin film geometry. In the metal case, a film thickness of five to ten atomic layers is usually sufficient to obtain bulk-like properties in the centre of the film and, consequently, true surface phenomena on the two film-vacuum interfaces. The

spin density functional theory described above provides an elegant and powerful framework to describe the electronic and magnetic structure of the surface. In its local approximation spin-density functional theory leads to Schrödinger-like one-electron equations containing an effective potential energy operator, which is determined by the self-consistent charge distribution. Thus the local spin-density functional one-particle equation has to be solved iteratively.

One of the most precise and powerful schemes to solve the local spin-density one-particle equation for the thin film geometry is the all-electron full-potential linearized augmented plane wave (AFLAPW) method [19].

The basic idea in this variational method is the partition of real space into three different regions, namely, spheres around the nuclei, vacuum regions on both sides of the film and the remaining interstitial region. In each of these regions the natural form of the variational basis functions are adopted. Firstly, in the interstitial region, plane waves are used; secondly, the product of the radial and spherical harmonics inside the spheres are adopted, whereas in the free space the product of the functions dependent only on the coordinate normal to the surface of the film and the plane wave are chosen.

Each of these basic functions is continuous in value and derivative across the various boundaries. This is possible because inside the sphere two radial functions for each l-value are used, and analogously in the vacuum two plane wave function are adopted.

In the AFLAPW method no shape approximation is needed to the charge density and the potential. Both the charge density and the effective one-electron potential are represented by the same analytical expansion described above, i.e., a Fourier representation in the interstitial region and an expansion in spherical harmonics inside the spheres and, in the vacuum, two-dimensional Fourier series in the set of planes parallel to the surfaces.

Generality of the potential requires a method to solve Poisson's equation for the density and potential without shape approximation. This is achieved by the new scheme proposed by Weinert [20]. The key idea in this new method is the observation that the potential outside a sphere depends only on its multipole moments. Now, the Poisson equation is solved straightforwardly when the charge density is given in Fourier representation. Because of the sharp structure of the charge density in the core regions, a Fourier expansion of the total density would be extremely slowly convergent. However, since the potential outside the sphere depends on the charge density inside only through the multipole moments, the true charge density can be replaced by a smooth density, which has a rapidly converging Fourier series and the same multipole moments as the true density. With this replacement of the density inside the spheres we have a Fourier expansion of the charge density giving the correct potential outside the sphere boundaries. To find the potential inside the sphere we are faced in the final step with a standard boundary-value problem of classical electrostatics which can be

solved from the original charge densities inside the sphere and on the sphere boundaries by the Green's function method.

For a thin film geometry the wave function for each state is a solution of the one-electron equation

$$[-\nabla^2 + V_{\text{eff}}(\vec{r})]\, \Phi_j(\vec{k}, \vec{r}) = E_j(\vec{k})\, \Phi_j(\vec{k}, \vec{r}), \tag{2.15}$$

where $\vec{k}$ is a vector of the two-dimensional first Brillouin zone and j is a band index. The effective potential, $V_{\text{eff}}(\vec{r})$, is given as the sum of the electrostatic Coulomb potential, related to the charge density by Poisson equation, and the local exchange and correlation potentials obtained by many-body theory [1].

In the AFLAPW method the wave function of each state is expanded variationally in reciprocal lattice

$$\Phi_i(\vec{k}) = \sum_j c_{ij}\, \Phi(\vec{k} + \vec{G}_j) \tag{2.16}$$

where each of the basis functions is an augmented plane wave given by

$$\Phi(\vec{K}_j) = \begin{cases} \sum_j [A_L(\vec{K}_j)\, u_l(E_l, \vec{r}) + B_L(\vec{K}_j)\, \dot{u}_l(E_l, \vec{r})]\; Y_L(\vec{r}); & r \in \text{sphere} \quad (2.17a) \\ (1/\Omega)^{1/2} \exp(i\vec{K}\vec{r}_j); & r \in \text{interstitial} \quad (2.17b) \\ \sum_j [A_q(\vec{K}_j)\, u_q(E_V, z) + B_q(\vec{K}_j)\, \dot{u}_q(E_V, z) \exp[i(\vec{k} + \vec{K}_q)\vec{r}]; & \\ & r \in \text{vacuum.} \quad (2.17c) \end{cases}$$

Here, Ω is the volume of the unit cell between the vacuum boundaries $\mp D/2$; the $u_l(E_l, \vec{r})$ are solutions of the radial Schrödinger equation obtained with the spherical part of the effective potential inside the sphere for a fixed energy E_l; and $\dot{u}_l(E_l, \vec{r})$ is the energy derivatives of this radial function. The coefficients $A_L(\vec{K}_j)$ and $B_L(\vec{K}_j)$ are determined by the requirements that the plane wave outside the sphere and the inside radial function is smoothly continued in value and derivative across the sphere boundaries. Similarly, in the vacuum the $u_q(E_V, z)$ are solutions of the equation

$$[-\delta^2/\delta z^2 + V(z) - E_V + (\vec{k} + \vec{K}_q)^2]\, u_q(E_V, z) = 0; \tag{2.18}$$

where $V(z)$ is the component of the effective potential in the vacuum, E_V is an energy parameter analogous to E_l inside the muffin-tin sphere, and $\dot{u}_q(E_V, z)$ is the energy derivative of the function $u_q(E_V, z)$. The matching coefficients $A_q(\vec{K}_j)$ and $B_q(\vec{K}_j)$ are determined by the continuity conditions of $\Phi(\vec{K}_j)$ across the vacuum boundaries $\mp D/2$.

Now the AFLAPW electronic charge density is represented in each of the three spatial regions by the following representation:

$$\rho(r)=\begin{cases}\sum_{i}\rho_i\exp(i\vec{G}_i\vec{r}) & r\in\text{interstitial} \quad (2.19a)\\ \sum_{L}\rho_L(\vec{r})\,Y_L(\vec{r}) & r\in\text{sphere} \quad (2.19b)\\ \sum_{q}\rho_q(z)\exp(i\vec{K}_q\vec{r}) & r\in\text{vacuum.} \quad (2.19c)\end{cases}$$

The electrostatic potential is obtained from the electronic charge density and nuclear charges by solving Poisson's equation.

The exchange and correlation potentials are calculated from the local electronic charge density. Finally, the effective one-electron potential as a sum of the electrostatic and exchange-correlation potential is represented in a form completely analogous to the charge density.

The one-particle equation with the effective potential are now solved iteratively. An initial density in the form given above is constructed from the superposition of self-consistent atomic densities. From these densities the corresponding potential is calculated, which defines the effective one-particle operator of the potential energy. Using the expansion for $\Phi_j(\vec{r})$ and the explicit form of the basic functions, the coefficients c_{ij} are obtained by Rayleigh-Ritz variational procedure. These coefficients now define the film wave function $\Psi_i(\vec{k})$ and give a new charge density

$$\rho(\vec{r})=e^2\sum_{\text{occup}}\Psi_i^*(\vec{k},\vec{r})\,\Psi_i(\vec{k},\vec{r})\,d^3r. \quad (2.20)$$

The density of the core electrons is obtained by solving fully relativistically a free atom-like problem using the effective potential. This completes one iteration cycle. The new density is fed back and self-consistency is achieved when the output density is approximately equal to the input density.

III. PRINCIPLES OF ELASTIC SPIN POLARIZED LOW ENERGY ELECTRON DIFFRACTION

The spin polarized low energy electron spectroscopic methods which are used to search for the electronic and magnetic structure of different solid state surfaces have in common that during the scattering process with the surface system an electron is added to or is removed from the system. From the theoretical point of view it means that in the scattering process with a surface, we are dealing with single particle excitation of an inhomogeneous many-electron system. To make this complicated many-body problem theoretically tractable, it is necessary to reduce it to an effective one-electron problem with several simplifying assumptions.

In elastic as well as in inelastic scattering by a surface, free polarized electrons are incident on the surface and after interaction during the scattering process there appear back scattered electrons which are employed to obtain information about the physical properties of the surface system.

It is well known that the spin polarization of an incident free electron beam is described by the polarization vector

$$P=\mathrm{tr}(\vec{\sigma}\hat{\rho})/\mathrm{tr}(\hat{\rho}) \tag{3.1}$$

where $\hat{\rho}$ is the statistical operator describing the electron beam and the vector $\vec{\sigma}$ stands for the 2×2 Pauli spin matrices

$$\sigma_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{3.2}$$

The quantity P is referred to as the degree of polarization. With respect to a given preferential direction $\hat{e}$, the polarization is

$$\vec{P}\cdot\hat{e}=(N^{\uparrow}-N^{\downarrow})/(N^{\uparrow}+N^{\downarrow}), \tag{3.3}$$

where $N^{\uparrow\downarrow}$ is the number of electrons with spin parallel ($\uparrow$) and antiparallel ($\downarrow$) to $\hat{e}$, respectively.

For a given incident beam of kinetic energy E, momentum $\vec{k}$ and polarization vector $\vec{P}$, the scattered electrons characterized by energy E', momentum $\vec{k}'$ and polarization vector $\vec{P}'$ gives us two possibilities:

1. Detection of the elastically scattered electrons with parameters $E'=E$, $\vec{k}'$ and $\vec{P}'$. This spectroscopy is known as elastic spin polarized low energy electron diffraction (E SPLEED).
2. Detection of outgoing electrons with energy $E'<E$, momentum $\vec{k}'$ and polarization vector $\vec{P}'$. This comprises inelastic electron scattering known as energy loss spectroscopy, Auge emission and true secondary electron emission (SEE).

Among the various surface spectroscopy methods involving low energy (up to about 200 eV) polarized free electrons elastic SPLEED is the simplest from the theoretical point of view.

In a SPLEED experiment, a monoenergetic beam of electrons of kinetic energy E and wave vector $\vec{k}$, with components $\vec{k}_{xy}$ parallel to the surface and $\vec{k}_z$ normal to it, is diffracted at the surface into beams with energy E and wave vectors $\vec{k}^{\vec{g}}_{xy}$ such that their components are given by

$$\vec{k}^{\vec{g}}_{xy}=\vec{k}_{xy}+\vec{g};\qquad \vec{k}^{\vec{g}}_{z}=[2E-(\vec{k}^{\vec{g}}_{xy})^2]^{1/2}, \tag{3.4}$$

where $\vec{g}$ denotes the two-dimensional surface reciprocal lattice vector. Momentum parallel to the surface is thus conserved modulo a surface reciprocal vector $\vec{g}$ due to the translation symmetry in the plane parallel to the surface. The beam with real $k^{\vec{g}}_z$ emerges from the surface and can be detected as propagating beams giving rise to spots on a fluorescent screen.

In standard low energy electron diffraction (LEED), maximal information on the surface is obtained by first measuring the intensities $I_{\vec{g}}$ of the diffracted beams as functions of the energy E and $\vec{k}$ which is usually characterized by the polar angle of incidence θ with respect to the surface normal $\hat{n}$ and the azimuthal angle φ, and then by comparing them to their theoretical counterparts calculated for

assumed surface structural models. The true surface structure is identified by optimal agreement between the experimental and theoretical results.

In elastic SPLEED one has the following basic observable quantities $I_{\vec{g}}(E, \theta, \varphi, P)$ and $\vec{P}_{\vec{g}}(E, \theta, \varphi, P)$, where $\vec{P}_{\vec{g}}$ denotes the polarization of the $\vec{g}$-th scattered beam and the meaning of the remaining parameters is the same as in standard LEED. If the surface is ferromagnetically ordered, a relativistic Hamiltonian describing the scattering process of the electron incident on the surface system can be expressed by means of the effective energy dependent electrostatic potential $V(E, \vec{r})$ and effective energy dependent magnetic field $\vec{B}(E, \vec{r})$, to be

$$H = c\vec{\alpha} \cdot \vec{p} + \beta mc^2 + V(E, \vec{r}) - \vec{\sigma} \cdot \vec{B}(E, \vec{r}), \tag{3.5}$$

where c is the velocity of light, m the electron rest mass, $e = -e$ the electron charge, while $\vec{\alpha} = (\alpha_x, \alpha_y, \alpha_z)$, and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are 4×4 Dirac matrices.

Denoting by $\hat{m}$ the unit vector in the direction of the magnetization of the surface and restricting our considerations to the case in which spin-orbit as well as the other relativistic corrections are small, we obtain the different surface scattering potentials for different directions of the magnetization

$$V_{\text{eff}}(E, \vec{r}) = V(E, \vec{r}) \mp \vec{B}(E, \vec{r}). \tag{3.6}$$

From the above one can see that spin effects in the scattering of spin-polarized low energy electron diffraction by the surface become manifested by reversal of the polarization of the incident beam as well as by reversal of the direction of the surface magnetization with respect to the unit vector $\hat{m}$. Thus we have to distinguish for each diffracted beam four intensities $I^m_{\vec{g}s}$, where $s = (\uparrow, \downarrow)$ refers to the directions of the primary beam polarization $\vec{P}$, and $m = (\uparrow, \downarrow)$ refers to the directions of the effective magnetic field $\vec{B}(E, \vec{r})$ parallel, and $-\vec{B}(E, \vec{r})$ antiparallel to the unit vector $\hat{m}$ of the preferential direction. The latter definition implies that $m = \uparrow$ is associated with the majority spin direction of the ferromagnet parallel to magnetization.

The four intensities $I^m_{\vec{g}s}$, which are the observables in experiment upon separate reversal of the incident polarization $\vec{P}$ and the effective magnetic field $\vec{B}$, are equivalent to their sum $I_{\vec{g}}$ and three scattering quantities defined as follows:

$$A1 = [(I^{\uparrow}_{\vec{g}\uparrow} + I^{\downarrow}_{\vec{g}\uparrow}) - (I^{\uparrow}_{\vec{g}\downarrow} + I^{\downarrow}_{\vec{g}\downarrow})]/I_{\vec{g}}, \tag{3.7}$$

$$A2 = [(I^{\uparrow}_{\vec{g}\uparrow} + I^{\downarrow}_{\vec{g}\downarrow}) - (I^{\uparrow}_{\vec{g}\downarrow} + I^{\downarrow}_{\vec{g}\uparrow})]/I_{\vec{g}}, \tag{3.8}$$

$$A3 = [(I^{\uparrow}_{\vec{g}\uparrow} + I^{\uparrow}_{\vec{g}\downarrow}) - (I^{\downarrow}_{\vec{g}\uparrow} + I^{\downarrow}_{\vec{g}\downarrow})]/I_{\vec{g}}. \tag{3.9}$$

These quantities describe the different asymmetries which correspond to the different interactions which have taken place during the scattering process. For a non-magnetic surface, the only relevant mechanism is spin-orbit coupling and $B = 0$, which implies that $I^{\uparrow}_{\vec{g}s} = I^{\downarrow}_{\vec{g}s} = I_{\vec{g}}$. In this case $A2 = A3 = 0$ and only $A1$ is non-zero giving

$$A1=(I_{\vec{g}\uparrow}-I_{\vec{g}\downarrow})/(I_{\vec{g}\uparrow}+I_{\vec{g}\downarrow}). \tag{3.10}$$

This is the well known spin-orbit induced asymmetry used in the Mott analyzer camera.

For a ferromagnetic surface the exchange term $(\vec{\sigma}\cdot\vec{B})$ reverses its sign changing the direction of the magnetic field. This implies that $I^{\uparrow}_{\vec{g}s}=I^{\downarrow}_{\vec{g}s}$ and since $A1$ contains for each spin direction s the sum $(I^{\uparrow}_{\vec{g}s}+I^{\downarrow}_{\vec{g}s})$, the exchange effects cancelling in $A1$ and the quantity $A1$ still leaves spin-orbit coupling as the dominant origin of the asymmetry in the intensities measured.

To discover the physical meaning of the other asymmetries, let us assume that spin-orbit coupling in the scattering under consideration can be ignored. In this case we can see that reversing simultaneously the directions of surface magnetization and polarization of the incident beam implies $I^{m}_{\vec{g}s}=I^{-m}_{\vec{g}-s}$ giving $A1=A3=0$ and the asymmetry $A2$ reduces to a purely magnetic exchange effect.

Let us observe that for each $m=\mathrm{sign}\,(\vec{\sigma}\cdot\vec{B})$, the sum $I^{m}_{\vec{g}\uparrow}+I^{m}_{\vec{g}\downarrow}$ corresponds to the scattered intensity due to the primary beam, which is an incoherent superposition of two oppositely polarized beams of the same intensity, and thus is equivalent to an unpolarized beam. This determines the physical meaning of the $A3$ asymmetry. It is an asymmetry obtained from an unpolarized incident beam scattered by a magnetic surface upon reversal of the magnetization direction.

The information about the surface magnetic properties coded in the experimental quantities described above, in order to be discovered and utilized in the understanding of surface magnetism, requires quantitatively realistic theoretical calculation assuming a reasonable structural model of the surface under consideration.

To do this it is convenient to express the observable quantities by means of a scattering matrix relating the plane wave four-spinor $\tilde{v}_{\vec{g}}$ which is the solution of the Dirac equation in vacuum and describes the scattered $\vec{g}$-th beam to the plane wave four-spinor $\tilde{u}$ describing incident electron beam. Because all the four components of the four plane wave spinor are not independent mutually and a transformation between the plane wave spinors is uniquely specified by transforming the two large components [1a], it suffices to have the two-dimensional scattering matrices $\hat{S}_{\vec{g}}$ for every scattered beam $\vec{g}$. This means that we have to look for the $\hat{S}_{\vec{g}}$ operator which acts in spin space and which operating on the free electron plane wave Pauli spinor, transforms it into another scattered plane wave Pauli spinor

$$\tilde{v}_{\vec{g}}=\hat{S}_{\vec{g}}\tilde{u}. \tag{3.11}$$

If the incident electron beam is not in a pure state $\tilde{u}$ but is polarized with polarization $P<1$ it has to be described by a statistical operator $\hat{\rho}$ [17]

$$\hat{\rho}=(1+\vec{P}\cdot\vec{\sigma})/2, \tag{3.12}$$

and to obtain the statistical operator describing the scattered beam $\hat{\rho}_{\vec{g}}$ we recall that a partially polarized beam is a statistical mixture of two beams completely polarized in two opposite directions. Taking this into account and using eq. (3.11), we can write

$$\hat{\rho}_{\vec{g}}(\vec{P}) = \hat{S}_{\vec{g}}(1 + \vec{P}\cdot\vec{\sigma})\hat{S}_{\vec{g}}^{+}. \tag{3.13}$$

For ferromagnetic surfaces the scattering operator $\hat{S}_{\vec{g}}$ and therefore $\hat{\rho}_{\vec{g}}$ depend on the effective magnetic field $\vec{B}$ and on the polarization degree of the incident beam P; therefore the relative intensity of the scattered $\vec{g}$-th beam is given by

$$I_{\vec{g}}(\vec{P}, \vec{B}) = \mathrm{tr}\,[\hat{\rho}_{\vec{g}}(\vec{P}, \vec{B})]/\mathrm{tr}\,[\hat{\rho}(P)]\,. \tag{3.14}$$

Thus we have shown that the theoretical calculation of the four measured quantities $I_{\vec{g}s}^{m}$ for a given diffracted beam reduces to the calculation of the scattering matrix $\hat{S}_{\vec{g}}$ for the surface scattering system under consideration.

The calculation of the scattering matrix in the SPLEED theory is a very difficult and complicated task, however. Due to the strong interaction between the incident electron and the ion cores in the surface, the scattering matrices for both elastic and inelastic scattering of electrons are about ten million times greater than for X-rays. The strong inelastic scattering effectively removes electrons from the incident or diffracted electron beams so that the elastically scattered fraction which contains the diffraction information that leaves the surface is only 1–5% of the total scattered intensity. The total reflectivity is low, of the order of 1%. The observed peak widths of the diffraction beams are broad, and there is a significant amount of multiple scattering. In spite of the multiple scattering events that complicate the scattering matrix calculation, the large inelastic scattering restricts backscattering to a few atomic layers at the surface and greatly reduces the contribution of multiple scattering to the total scattered intensity.

At present the simplest approach to the scattering matrix calculation is that which uses the T-matrix formalism developed by Beeby [21] and extended by Duke and Tucker [22] to include inelastic damping of the electron beam. The outgoing beams each correspond to the two-dimensional reciprocal lattice vector, $\vec{g}$, in the plane of the surface, and we consider only the elastic scattering case where E represents the incident and emerging electron energy. The number of electrons scattered elastically into the beam labelled by $\vec{g}$ is proportional to the scattering cross section, $\sigma_{\vec{g}s}^{m}(E, \theta, \varphi)$

$$\sigma_{\vec{g}s}^{m} = (m^2/4\pi^2\hbar^4)[I_{\vec{g}s}^{m}(E, \vec{k}', \vec{k})]^2\,, \tag{3.14a}$$

where the intensity $I_{\vec{g}s}^{m}$ is given in terms of the T-matrix as follows:

$$I_{\vec{g}s}^{m}(..) = \frac{4\pi^2}{A}\delta(\vec{k}'_{xy} - \vec{k}_{xy} - \vec{g})\sum_{v}\exp[i(\vec{k} - \vec{k}')\vec{d}_v]\, T_{vs}^{m}(E, \vec{k}', \vec{k}). \tag{3.15}$$

The vector $\vec{d}_v$ gives the position of the origin in the v-th layer with respect to the origin in the surface layer and A is the area of the unit cell in a plane parallel to the surface. The delta function expresses the condition for the existence of the diffraction beams and $T^m_{vs}(E, \vec{k}', \vec{k})$ is the transition T-matrix for scattering of an incident electron by the v-th layer in the presence of the other layers of the surface.

The expression obtained for the measured intensities $I^m_{\vec{g}s}$ shows that the crucial quantities in SPLEED theory which have to be calculated, are just the matrix elements of $T^m_{vs}(E, \vec{k}', \vec{k})$ for which we can use as a starting point the operator equation for the $\hat{T}$-operator, i.e., the Dyson equation

$$\hat{T} = \hat{V}_{\text{eff}} + \hat{V}_{\text{eff}} \hat{G}_0 \hat{T} \tag{3.16}$$

in which $\hat{G}_0$ denotes the free-electron Green function operator and $\hat{V}_{\text{eff}} = \hat{V}$ denotes any reasonable one-electron surface scattering potential operator which has to be specified for a given surface. This will be done in the next section.

Now without knowing the explicit form of the spin dependent surface scattering potential we can solve the above equation in operator symbolic form. To do that let us decompose the scattering potential operator $\hat{V}$ as well as the scattering operator $\hat{T}$ in sums of atomic-like terms as follows:

$$\hat{T} = \sum_{\vec{vj}} \hat{T}_{\vec{vj}}, \qquad \hat{V} = \sum_{\vec{vj}} \hat{V}_{\vec{vj}}. \tag{3.17}$$

Inserting this into the Dyson equation we have

$$\sum_{\vec{vj}} \hat{T}_{\vec{vj}} = \sum_{\vec{vj}} \hat{V}_{\vec{vj}} + \sum_{\vec{vj}} \hat{V}_{\vec{vj}} \hat{G}_0 \sum_{\vec{v'j'}} \hat{T}_{\vec{v'j'}} \tag{3.18}$$

where $\vec{vj}$, $\vec{v'j'}$ label the surface atomic sites in the surface, i.e., v or v' labels the monoatomic layer parallel to the surface plane, and $\vec{j}$ or $\vec{j}'$ the positions of the atoms in a given layer.

A decomposition like this allows us to write the Dyson equation for the single site transition operator $\hat{T}_{\vec{vj}}$

$$\begin{aligned} \hat{T}_{\vec{vj}} &= \hat{V}_{\vec{vj}} + \hat{V}_{\vec{vj}} \hat{G}_0 \hat{T}_{\vec{vj}} + \hat{V}_{\vec{vj}} \hat{G}_0 \sum_{\vec{vj} \neq \vec{v'j'}} \hat{T}_{\vec{v'j'}} \\ &= \hat{V}_{\vec{vj}} (1 + \hat{G}_0 \hat{T}_{\vec{vj}}) = \hat{t}^{\vec{vj}} (1 + \hat{G}_0 \sum_{\vec{vj} \neq \vec{v'j'}} \hat{T}_{\vec{v'j'}}), \end{aligned} \tag{3.19}$$

where we have defined the new scattering matrix for vj-th site

$$\hat{t}^{\vec{vj}} = \hat{V}_{\vec{vj}} + \hat{V}_{\vec{vj}} \hat{G}_0 \hat{t}^{\vec{vj}}. \tag{3.20}$$

Now, on iteration of the last equation of (3.19) we have the following result:

$$\hat{T} = \sum_{\vec{vj}} \hat{t}^{\vec{vj}} + \sum_{\vec{vj}} \hat{t}^{\vec{vj}} \hat{G}_0 \sum_{\vec{v'j'} \neq \vec{vj}} \hat{t}^{\vec{v'j'}} + \sum_{\vec{vj}} \hat{t}^{\vec{vj}} \hat{G}_0 \sum_{\vec{v'j'} \neq \vec{vj}} \hat{t}^{\vec{v'j'}} \hat{G}_0 \sum_{\vec{v''j''} \neq \vec{v'j'}} \hat{t}^{\vec{v''j''}} + \dots \tag{3.21}$$

and for the single site transition operator $\hat{T}_{v\vec{j}}$ we have

$$\hat{T}_v = \hat{t}^{v\vec{j}}\Big(1 + \hat{G}_0 \sum_{v'\vec{j}' \neq v\vec{j}} \hat{t}^{v'\vec{j}'} + G_0 \sum_{v'\vec{j}' \neq v\vec{j}} \hat{t}^{v'\vec{j}'} \hat{G}_0 \sum_{v''\vec{j}'' \neq v'\vec{j}'} \hat{t}^{v''\vec{j}''} \cdot + \ldots \cdot \tag{3.22}$$

The series (3.21) may be understood as follows. The first term on the right-hand side represents the electron being scattered from one of the potentials and then leaving the surface; the second term represents a scattering process at the site $v\vec{j}$, followed by a second scattering at a $v'\vec{j}'$ site of the surface; the higher terms represent higher order scattering, the only restriction being that no two successive scatterings shall be off the same atom site.

IV. SPIN DEPENDENT SCATTERING POTENTIAL AND SURFACE SCATTERING POLARIZATION FORMULAE

In order to write the effective spin dependent surface scattering potential for spin polarized incident electrons scattered from a magnetic surface we treat the latter as a thin film composed of several monoatomic layers parallel to the surface of a semi-infinite bulk crystal. Assuming that the monoatomic layers are (110) nickel crystal planes of f.c.c. structure, meaning that the magnetization of the sample with a free surface from which the incident electrons are scattered is parallel to the surface, the polarization effect measured in experiment [13] can be dealt with as an asymmetry effect in the scattering of the incident electrons with up (↑) and down (↓) spin directions and is an exchange interaction effect only, because in this experimental case the spin-orbit interaction effect is negligible.

We label the monoatomic layers parallel to the surfaces in the thin film by v ($v = 1, 2, \ldots n$), where $v = 1$ denotes the free monoatomic surface layer of the film while $v = n$ denotes the last considered monoatomic layer of the semi-infinite crystal. We denote by $\vec{j}$ the position of an atom in a given layer, say v, so that the positions of the thin film atoms can be described by the position vector $\vec{R}_{v\vec{j}} = \vec{j}_v + d_v \cdot \hat{e}$ where d_v denotes the normal distance of the v-th layer from the free surface layer of the crystal and $\hat{e}$ is the unit vector in the direction perpendicular to the surfaces and is directed inside the film.

Denoting by $V_T(\vec{r} - \vec{R}_{v\vec{j}}, \uparrow\downarrow)$ the effective scattering potential produced by the $(v\vec{j})$-th atom in the presence of other atoms of the thin film and the substrate for different spin directions of the incident electron we can write the total scattering potentials as [1b]

$$V_T(\vec{r}, \uparrow\downarrow) = \sum_{v\vec{j}} [V_T^{\text{Coul}}(\vec{r} - \vec{R}_{v\vec{j}}) \pm V_T^{\text{exc}}(\vec{r} - \vec{R}_{v\vec{j}})], \tag{4.1}$$

where the index T serves to point out that we are considering a temperature dependent scattering potential which, for a given static potential of the $(v\vec{j})$-th atom $V_0(\vec{r} - \vec{R}_{v\vec{j}})$, is defined by

$$V_T(\vec{r}-\vec{R}_{v\vec{j}},\uparrow\downarrow)=(2\pi B_v)^{-3/2}\int d^3r' V_0(\vec{r}'-\vec{R}_{v\vec{j}},\uparrow\downarrow)\exp\left[-\frac{|\vec{r}'-\vec{r}|^2}{2B_v}\right] \tag{4.2}$$

and where B_v stands for the mean-square displacement of the $(v\vec{j})$-th atom from its equilibrium position in thin film and is the same for all atoms in the same layer $(B_{v\vec{j}}=B_v)$.

In eq. (4.1) we understand that the spin independent part of the exchange term

$$\tfrac{1}{2}[V_T^{\mathrm{exc}}(\vec{r}-\vec{R}_{v\vec{j}},\uparrow)+V_T^{\mathrm{exc}}(\vec{r}-\vec{R}_{v\vec{j}},\downarrow)] \tag{4.3}$$

of the scattering potential has been included into the Coulomb term of the scattering potential of the $(v\vec{j})$-th atom $V_{v\vec{j}}^{\mathrm{Coul}}(\vec{r}-\vec{R}_{v\vec{j}})$ and thus $V_{v\vec{j}}^{\mathrm{exc}}(\vec{r}-\vec{R}_{v\vec{j}})$ denotes the spin dependent part of the exchange potential of the $(v\vec{j})$-th atom. It is now obvious that the effective scattering potential is different for the two spin directions of the incident beam, as we have pointed out previously.

We have shown earlier [1b] that if we do not prefer the decomposition into infinite series of the hyperbolic sine function which comes from integration in eq. (4.2) over the angles, we obtain another much more complicated form of the effective scattering potential by comparison with those used by us in [1] to compute the spin dependent scattering amplitude. However, we are now able to do the same with both equivalent forms of the potential; hence in our present work, we prefer the highly complicated form of the scattering potential because it leads to a simpler form of the scattering amplitude.

Let us write the expressions obtained for the Coulomb and exchange term of the $(v\vec{j})$-th atom scattering potential in their final forms:

$$V_T^{\mathrm{Coul}}(\vec{r}-\vec{R}_{v\vec{j}})=\frac{e\Phi\left(\dfrac{|\vec{r}-\vec{R}_{v\vec{j}}|}{2B_v}\right)}{|\vec{r}-\vec{R}_{v\vec{j}}|}\left[Z-\tfrac{1}{2}\sum_j\langle n_v^j\rangle G_j(|\vec{r}-\vec{R}_{v\vec{j}}|)\right] \tag{4.4}$$

$$V_T^{\mathrm{exc}}(\vec{r}-\vec{R}_{v\vec{j}})=\frac{e\Phi\left(\dfrac{|\vec{r}-\vec{R}_{v\vec{j}}|}{2B_v}\right)}{|\vec{r}-\vec{R}_{v\vec{j}}|}\sum_j\langle dn_v^j\rangle G_j(|\vec{r}-\vec{R}_{v\vec{j}}|) \tag{4.5}$$

where we have introduced the function $G_j(|\vec{r}-\vec{R}_{v\vec{j}}|)$, defined as follows:

$$G_j(|\vec{r}-\vec{R}_{v\vec{j}}|)=1+\frac{\exp(b_j^2B_v/4)}{\Phi(|\vec{r}-\vec{R}_{v\vec{j}}|/2B_v)}\sum_{m=0}^{a_j-1}(b_jB_v)^m\left(1-\frac{m}{a_j}\right)$$
$$\cdot[\hat{D}_{-(m-1)}(+)-\hat{D}_{-(m+1)}(-)] \tag{4.6}$$

where the operator $\hat{D}_{-m}(...)$ denotes the shorthand notation for the right-hand side of the following equation:

$$\hat{D}_{-m}(\ )=\exp\left[-\frac{|\vec{r}-\vec{R}_{v\vec{j}}|^2}{4B_v}\pm\frac{b_j|\vec{r}-\vec{R}_{v\vec{j}}|}{2}\right]D_{-m}\left(b_jB_v\pm\frac{|\vec{r}-\vec{R}_{v\vec{j}}|}{B_v}\right) \tag{4.7}$$

and where $D_{-m}(...)$ is the standard parabolic cylindrical function and can be expressed by means of the erf(x) function defined by

$$\mathrm{erf}(x)=\Phi(x)=\frac{2}{\sqrt{\pi}}\int_0^x dt\exp(-t^2). \tag{4.8}$$

In the above, the parameters a_j and b_j are numerical parameters for the j-th Slater orbital of a free atom [23]; $\langle n_v^j\rangle$ denotes the thermodynamically averaged occupation numbers of the j-th orbitals of atoms in the v-th monoatomic layer, while by $\langle dn_v^j\rangle$ we have denoted the difference between the down and up electron occupation numbers for the given j-orbital of the v-th atom in the film under consideration. For these quantities we assume that they are known from thin film self-consistent theory [3].

Having the explicit expressions for both the Coulomb and exchange terms of the surface scattering potential, we can compute the scattering amplitude $f_T(K,\uparrow\downarrow)$ in the first Born approximation [1]. We use $\vec{K}$ to denote the scattering vector. The final results obtained for the scattering amplitude will be written here for up ($\uparrow$) and down ($\downarrow$) spin directions of the incident electron beam separately:

$$f_T(K,\uparrow)=F_{\parallel}(\vec{K}_{\parallel})\sum_{v=1}^{n}\exp(-iK_{\perp}d_v-\tfrac{1}{2}K^2B_v)\cdot\frac{2me^2}{\hbar^2K^2}\left[Z-\tfrac{1}{2}\sum_{j=1}^{4}(\langle n_v^j\rangle-\langle dn_v^j\rangle)Z_j(K,a_j,b_j)\right], \tag{4.9}$$

$$f_T(K,\downarrow)=F_{\parallel}(\vec{K}_{\parallel})\sum_{v=1}^{n}\exp(-iKd_v-\tfrac{1}{2}K^2B_v)\cdot\frac{2me^2}{\hbar^2K^2}\left[Z-\tfrac{1}{2}\sum_{j=1}^{4}(\langle n_v^j\rangle+\langle dn_v^j\rangle)Z_j(K,a_j,b_j)\right], \tag{4.10}$$

where the exponential factor occurring in the above equations is the Debye-Waller factor of the v-th layer atoms. The quantity $F_{\parallel}$ is the two-dimensional structure factor of the thin film under consideration and is given by:

$$F_{\parallel}(\vec{K}_{\parallel})=(1/nN^2)\sum_j\exp(-i\vec{K}_{\parallel}\vec{j}_v), \tag{4.11}$$

nN^2 being the number of atoms in the thin film, while $\vec{K}_{\parallel}$ and $\vec{K}_{\perp}$ denote components of the scattering vector $\vec{K}$ parallel and perpendicular to the film surface, respectively. The function $Z_j(K,a_j,b_j)$ appearing in eqs. (3.10 and 3.11) is given by

$$Z_j(K,a_j,b_j)=1-\sum_{m=0}^{a_j-1}(1-m/a_j)\left(\frac{1}{1+K^2/b_j^2}\right)^{m+1}\cdot\sum_{0<2k<m}(-1)^k\binom{m+1}{2k+1}(K^2/b_j^2)^{k+1}, \tag{4.12}$$

where a_j and b_j are numerical parameters; they are given for all elements in Gombas and Szondy's paper [23].

This new form of the surface scattering amplitude is much simpler than those obtained in our previous papers [1]; we shall use it to compute the polarization effect of the spin direction dependent electron beams scattered from Ni(110) surfaces.

The relative current P measured in the SPLEED experiment described in [13] is given by

$$P(K)=\frac{\dfrac{d\sigma(\uparrow)}{d\Omega}-\dfrac{d\sigma(\downarrow)}{d\Omega}}{\dfrac{1}{2}\left[\dfrac{d\sigma(\uparrow)}{d\Omega}+\dfrac{d\sigma(\downarrow)}{d\Omega}\right]}=A2_T(K). \tag{4.13}$$

Here $K=|\vec{K}|=2k_0|\sin(\frac{1}{2}\theta)|$; k_0 denotes the incident electron wave vector, θ the scattering angle and $d\sigma(\uparrow\downarrow)/d\Omega$ is the scattering differential cross-section related with the scattering amplitude by way of the following formula

$$\frac{d\sigma(\uparrow,\downarrow)}{d\Omega}=|f_T^{\uparrow\downarrow}(K)|^2. \tag{4.14}$$

Inserting the explicit form of the respective amplitudes given by eqs. (4.10–4.12) into (4.13) and using the relation (4.14), we obtain the exchange asymmetry formula

$$A2_T(K)=\frac{\sum_{vv'}\exp(-iKd_{vv'}-\frac{1}{2}K^2B_{vv'})\,2\,[Z_{v'}^{\mathrm{Coul}}(K)\,Z_v^{\mathrm{exc}}(K)+Z_{v'}^{\mathrm{Coul}}(K)\,Z_v^{\mathrm{exc}}(K)]}{\sum_{vv'}\exp(-iKd_{vv'}-\frac{1}{2}K^2B_{vv'})\,[Z_v^{\mathrm{Coul}}(K)\,Z_{v'}^{\mathrm{Coul}}(K)+Z_v^{\mathrm{exc}}(K)\,Z_{v'}^{\mathrm{exc}}(K)]}. \tag{4.15}$$

When deriving this relation, we have used the following notation:

$$d_{vv'}=d_v-d_{v'};\qquad B_{vv'}=B_v+B_{v'}, \tag{4.16}$$

$$Z_v^{\mathrm{Coul}}(K)=Z-\sum_j\langle n_v^j\rangle\,Z_j(K,a_j,b_j)-\tfrac{1}{2}[\langle n_v^{d\uparrow}\rangle+\langle n_v^{d\downarrow}\rangle]\,Z_d(K,a_j,b_j), \tag{4.17}$$

$$Z_v^{\mathrm{exc}}(K)=\tfrac{1}{2}\langle dn_v^d\rangle\,Z_d(K,a_d,b_d), \tag{4.18}$$

$$\langle dn_v^d\rangle=\langle n_v^d(\uparrow)\rangle-\langle n_v^d(\downarrow)\rangle. \tag{4.19}$$

Here, index d ($j=3$) is used for the d-band electrons. Another thing which we have to note is that the above relations are written in the one-band approximation (d-band). In this case only the quantities $\langle dn_v^d\rangle$ for different monoatomic layers parallel to the surfaces of the thin film have to be known from self-consistent band calculations.

Now it is clearly seen that if we replace all effective scattering parameters describing the scattering of v-th layer atoms in the surface by an averaged parameter, the same for each layer in the surface, the asymmetry $A2_T(K)$ reduces to

$$A2_T(K)=\frac{\langle dn_T^d(n)\rangle\,Z_d^{\mathrm{exc}}(K)}{Z^{\mathrm{Coul}}(K,n)}, \tag{4.20}$$

where n stands for the number of monoatomic layers parallel to the surface penetrated by incident electrons during the scattering process. However, in a standard SPLEED experiment with an incident electron beam of energy up to 90 eV the mean free path of the electrons in the nickel crystal is about 5 Å and thus the electron penetration depth is only 2.5 Å. This means that in SPLEED experiments we can measure an exchange asymmetry caused by one and a half monoatomic layers. Supposing that the approximation leading from the formula (4.15) to (4.20) is reasonable, we have an explicit proportionality relation between the exchange asymmetry on reversal of the incident beam polarization and the mean magnetization of the surface.

V. NUMERICAL RESULTS AND CONCLUSIONS

To compute the polarization asymmetry effect of electron scattering from magnetic surfaces by means of the general formula (4.15) we have to use trial and error interaction between the theory and experiment, as usually in LEED. This is so because the surface parameters B_v and $\langle dn_v \rangle$ are not known. Especially, their temperature dependence as well as their distribution in the direction perpendicular to the surface require self-consistent solution of the many-body problem described in Section II. Additionally, the self-consistent solution has to be known for temperatures in the range from zero to critical. This is not possible at present and the discussion of the exchange asymmetry formula (4.15) obtained has to be restricted to its special cases for which the above mentioned distributions are available.

We have calculated the relative exchange asymmetry on the momentum transfer K for fully polarized Ni surface (at $T=0$ K) by means of the approximated formula (4.20). In this case we have

$$A2(K, n) = \langle dn(n) \rangle Z_d^{\mathrm{exc}}(K, a_d, b_d)/Z^{\mathrm{Coul}}(K, n). \tag{5.1}$$

The results obtained for the surface in the model of Jepsen *et al.* [26], in which the numbers of d-electrons with up and down spin directions are known for the topmost monoatomic layers (their difference is shown in Fig. 2) are presented in Fig. 1, where we have shown additionally Saldana and Helman's results for bulk nickel [24b] obtained by using the self-consistent Wakoh potential [24a]. One notes that our results coincide with those of Saldana and Helman if the surface is treated as a film of $n=3$ topmost monoatomic layers.

To bring the general formula (4.15) into contact with the SPLEED experiments we have used three surface magnetization models at $T=0$ K for which layer-dependent magnetization extrapolated to some experimental temperatures are known [25–27].

The models are illustrated in Figs. 2–4 for three temperatures: $T=0$ K, $T=300$ K, and $T=520$ K. In these figures we have showed the distributions of the

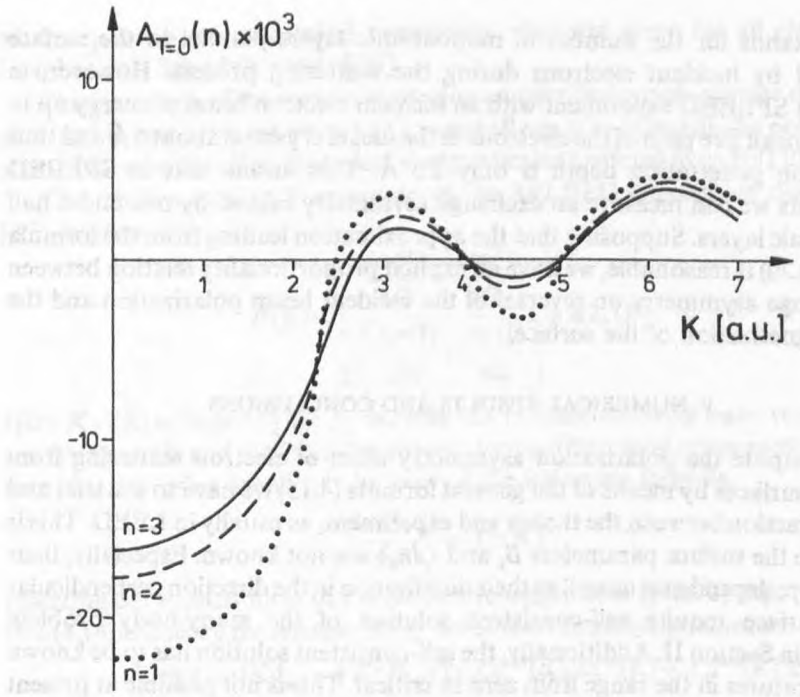

Fig. 1. The exchange asymmetry computed by means of eq. (5.1) at $T=0$ K as a function of the momentum transfer K, for the nickel surface treated as a thin film with a number n of the topmost monoatomic layers in the case of the Jepsen *et al.* [26] surface magnetization model. For $n=3$ our results coincide with those of Saldana and Helman [24b] (full line).

parameters $M_v \sim \langle dn_v \rangle$ of the monoatomic layers parallel to the surface at the three temperatures. They are necessary to the calculation of the polarization effects by means of eq. (4.15). Using these quantities we have computed the relative exchange asymmetry $A2(T)/A2(0)$ for the Ni(110) surface. This surface has been chosen principally because there exist experimental results for it in the temperature range from 0.5 to $0.8T/T_c$ and, moreover, because in the case of Ni(110) surfaces SPLEED experiments measure the true exchange asymmetry without spin-orbit coupling, as we have already mentioned.

To calculate the relative asymmetry, the spacing between the first and the second top layer has been assumed to be 1% larger than in the bulk. The other layer spacing are treated as the same as the bulk ones.

The layer dependent mean square displacements in terms of which we have expressed the temperature scattering potential, and which consequently occur in the formula (4.15), have been calculated numerically by us applying a formalism described elsewhere [28] in connection with the standard LEED problem without spin polarization of the incident electron beam.

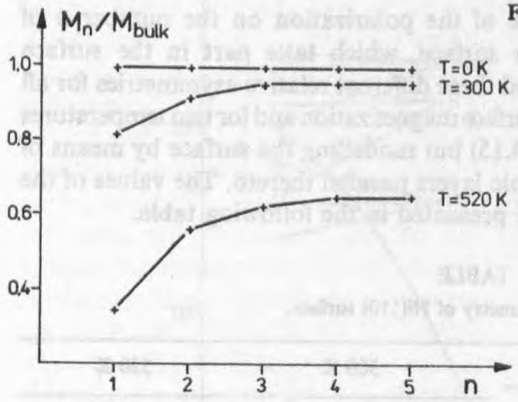

Fig. 2. The homogeneous layer dependent surface magnetization model [25].

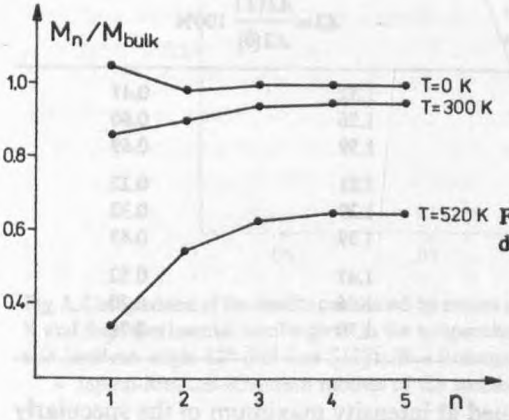

Fig. 3. The Jepsen-Madsen-Andersen layer dependent surface magnetization model [26].

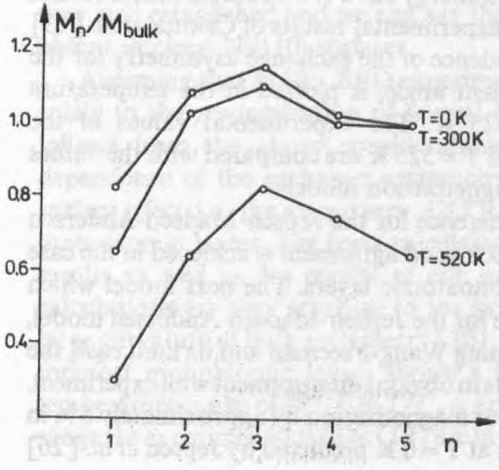

Fig. 4. The Wang-Freeman layer dependent surface magnetization model [27].

To demonstrate the dependence of the polarization on the number n of monoatomic layers parallel to the surface, which take part in the surface scattering process, we have calculated three different relative asymmetries for all three models of the layer-dependent surface magnetization and for two temperatures (300 and 520 K), always using eq. (4.15) but modelling the surface by means of $n=1, 2, 3$ of the topmost monoatomic layers parallel thereto. The values of the exchange asymmetries obtained are presented in the following table.

TABLE

Exchange asymmetry of Ni(110) surface.

Temperature		300 K	520 K
Surface model	n	Exchange asymmetry $A2=\frac{A2(T)}{A2(0)}100\%$	
1. Homogeneous model	1	1.32	0.47
	2	1.56	0.60
	3	1.59	0.69
2. Wang-Freeman	1	1.21	0.22
	2	1.29	0.32
	3	1.39	0.43
3. Jepsen-Madsen-Andersen	1	1.47	0.52
	2	1.66	0.70
	3	1.70	0.78

The preceding results were obtained at intensity maximum of the specularly reflected (00) beam at an angle of 12° and energy 125 eV. To compare these results with experiment we have included the experimental results of Celotta *et al.* [13] in Fig. 5, where the temperature dependence of the exchange asymmetry for the same beam, electron energy and incident angle, is plotted in the temperature range approximately from 314 to 525 K. The experimental values of the asymmetry at temperatures $T=314$ and $T=525$ K are compared with the values presented in the Table for various magnetization models.

The comparison shows a clear preference for the Jepsen-Madsen-Andersen model of surface magnetization for which good agreement is achieved in the case of the surface modelled by $n=1$–2 monoatomic layers. The next model which gives an asymmetry very close to those for the Jepsen-Madsen-Andersen model, is the homogeneous model. The remaining Wang-Freeman and its limit case, the so-called dead layer model, lead to results in obvious disagreement with experiment.

The enhancement of the surface layer magnetization by approximately 5% in comparison to the bulk magnetization at $T=0$ K predicted by Jepsen *et al.* [26]

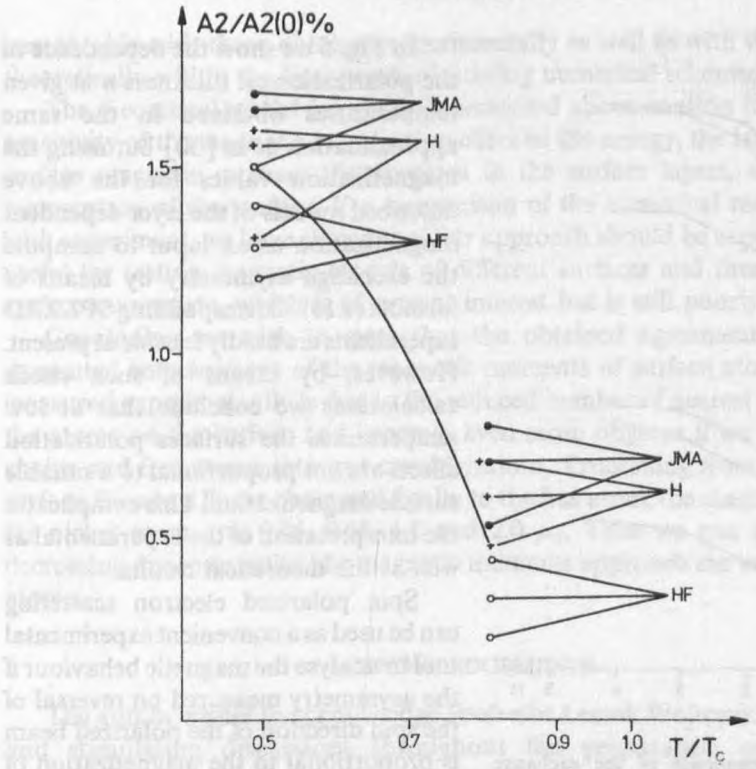

Fig. 5. Comparison of the results calculated by means of eq. (4.15) at the temperatures $T = 300$ and 520 K and the experimental results given in the temperature range of (0.5–0.8) T/T_c for energy $E = 125$ eV and incident angle 12° (full line [13]); H – homogeneous, WF – Wang and Freeman and JMA – Jepsen-Madsen-Andersen models of the surface magnetization distribution, respectively.

has also been found in self-consistent calculations by Freeman [29]; thus it is now well established and we can say that magnetic "dead layers" are definitely absent in clean Ni(110) surfaces.

Assuming that in SPLEED experiments the measured asymmetry $A2$ is due solely to the magnetization of several topmost surface layers, as it obviously follows from the above considerations, we focus now on the temperature dependence of the exchange asymmetry. The temperature dependence of the surface effect, i.e., the asymmetry $A2(T)/A2(0)$ for surfaces of different number of monoatomic layers, has been calculated by us in a previous paper [30]. The results as well as the results of our present paper prove that the SPLEED calculations are very sensitive to the surface magnetization. In contrast to the large curvature of bulk asymmetry [30], the surface exchange asymmetry for the topmost monoatomic layers shows a temperature dependence which in the temperature range of (0.5–0.8) T/T_c, is approximately linear. In this temperature range the experimental results [13] are in agreement with our calculations (Fig. 5).

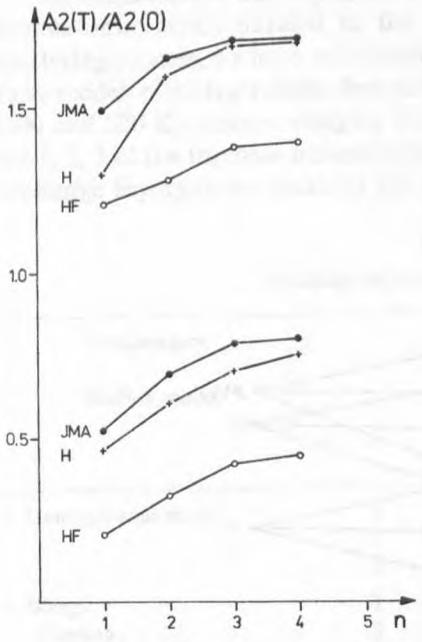

Fig. 6. The dependence of the exchange asymmetry on the number n of monoatomic layers used in the calculations for the three surface magnetization models at temperatures 300 and 520 K. Notation and other parameters as in Fig. 5.

In Fig. 6 we show the dependence of the polarization *vs.* thickness n at given temperatures obtained in the same approximation as in [30] but using the magnetization values for the above described models of the layer dependent magnetization as an input to compute the exchange asymmetry by means of formula (4.15). Corresponding SPLEED experiments are hardly feasible at present. However, by means of such check calculations we conclude that at low temperatures the surfaces polarization effects are not proportional to a suitable surface magnetization. This complicates the interpretation of the experimental as well as the theoretical results.

Spin polarized electron scattering can be used as a convenient experimental tool to analyse the magnetic behaviour if the asymmetry measured on reversal of the spin direction of the polarized beam is proportional to the magnetization of the first monoatomic layer parallel to the surface. This proportionality, as far as we know, could not be expected in general outside the critical region of temperature. However, at temperature near T_c, where the influence of the deeper placed atomic magnetic moments on the topmost monolayer atoms grows small with temperature, and is zero at $T = T_c$, the information depth of the low energy electrons comes to be closer to the true monoatomic surface of the crystal and one can therefore expect that the polarization effects of the diffracted electron beam is proportional to the surface magnetization.

VI. FINAL REMARKS

While in spin-orbit SPLEED good agreement has been achieved between theory and experiment [2], magnetic SPLEED is still in an earlier stage of development and quantitative comparisons could not as yet be made. However, we have shown that our analytical approach to the magnetic SPLEED problem used in the present paper to test Ni((110) surfaces leads to reasonable results

comparable with those obtained experimentally as well as with those obtained theoretically within the framework of existing numerical schemes and theories.

The theoretical model calculations presented above confirm the remarkable sensitivity of the magnetic polarization effect to the energy, the layer dependent surface magnetic moment distributions in the surface layers, as well as the temperature of the surface. *Via* comparison of the numerical results obtained with experiment, we have shown that our approach should be expected to prove useful for testing magnetic models of different surfaces and thus for studying surface magnetism, which is of current interest but is still poorly known.

Concluding we wish to state that the obtained agreement between the computed enhancement of the magnetic moments of surface atoms and those measured experimentally is due to the reduced number of nearest neighbours of the atoms on the surface and becomes even more obvious if we include linear chains and free atoms into our considerations. Proceeding from bulk to (110) surface, then to a linear chain and finally to the free atom, the magnetic moments for nickel atom are: 0.56, 0.68, 1.1 and 2.0 μ_B. Thus we can say that, with decreasing dimensionality, the magnetic moments approach the value of the free atoms.

ACKNOWLEDGEMENTS

The author wishes to acknowledge Professor Leszek Wojtczak for his fruitful and stimulating discussions throughout the preparation of this paper.

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